Path derivation for a wave scattered model to estimate height correlation function of rough surfaces

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The long standing problem on finding the height correlation function is studied by the inverse scattering problem. We propose a new method in the frame work of Kirchhoff theory which we call "path derivation of scattered wave (PDSW)" in order to obtain an expression for direct measurements of the height correlation function. This would provide adequate insight to rough surfaces. The efficiency of this method is due to the fact that the height correlation function could be estimated directly by measurements of the scattered intensity on a suggested path. The model is tested numerically and an experimental setup is suggested.

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The importance of rough surfaces in various fields of science and engineering has been highlighted by many researchers. The area of study spans from Biology [1], Polymer [2] and Radio [3] Science, Material engineering [4], and Physics (see [5] and references therein), etc. This motivates researchers specially in Physics to study the various aspects rough surfaces. The stick slip dynamics of rough surfaces was studied experimentally [6] for two surfaces where a hydrodynamic model was implemented to theoretically study the effects of surface roughness on viscous incompressible liquids [7]. Palasantzas studied the effect of roughness on ballistic thermal conductance of a nanosized beam [8] in addition to effects of the roughness exponent on friction while a viscous rubber slips in to a rough surface [9]. In a detailed study Volokitin and Persson [10] stated that if surface modes for instants adsorbate vibration modes exist on a surface, thermal radiation would be coherent and due to the electromagnetic oscillations on the surface, radiative heat transfer would be experienced.

The topography of any surface could be obtained by mechanical devices such as scanning probe microscopy, SPM [11, 12] e.g. in application to semiconducting carbon nanotube transistors [13]. But despite the wide range of applicability and benefits of SPM, the tip convolution may still remain as the main challenge for SPM [14], in addition to the limitations that SPM has in changing the scale of scanning. Optical techniques would overcome this limitation without scratching the surface. Optical techniques could also manage to determine the scale of observation with the incident light wave-length. The mostly implemented method in the optical technique is the scattering method where the roughness would play a major role on the scattering of waves [15]. Interesting work in the context of wave scattering has been car-

ried out in application to Brewster's scattering angle [16] and the Rayleigh hypothesis [17]. Since the wave-length could be either smaller or greater than the height fluctuations, the two scale theory was proposed [18]. In a further study, effects of interference of two beam scattering was considered [19]. All these plus the fact that studying the scattered wave would provide very useful information about the surface itself [20], would motivate studying the inverse scattered problem.

Inverse scattering techniques were implemented [21– 25] to measure the statistical properties of rough surfaces. Although after quite a long time since optical techniques were born, and many parameters like; root mean square of height [26], probability density function (PDF) [27], correlation length [28] etc. where estimated, not much progress has been achieved in order to find the most important parameter of the surface which is the height correlation function. This issue is the main aim of this work. The framework implemented is wave scattering by Kirchhoff theory approach [15, 29–31]. The Kirchhoff theory is an electromagnetic theory which treats any point on a scattering surface as a part of an infinite plane, parallel to the local surface tangent [15]. In this work a model is proposed to estimate the height correlation function of a random surface which we name; "path derivation of scattered wave". Taking into account this model enables experimentalists to obtain the height correlation function simply by only measuring the intensity of the scattered light in a special path. This technique would dramatically simplify the estimation of the height correlation function due to the fact that only one parameter (the scattered intensity) needs to be measured.

In Kirchhoff theory, the field of incident monochromatic wave may be written as $\psi^{inc}(r) = \exp(-ik_{inc}.r)$, where k and r indicate the wave number and position re-

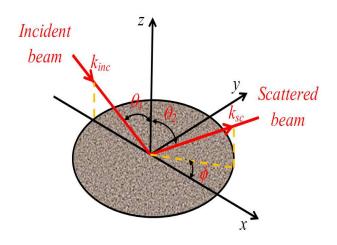


FIG. 1: The geometry used for wave scattering from a rough surface.

spectively. In Fig. 1 a beam is shown incident to a rough surface with dimensions $-X \leq x_0 \leq X$, $-Y \leq y_0 \leq Y$ with a reflection coefficient R_0 equal to -1 corresponding to the Dirichlet boundary condition. The total scattered field over the mean reference plane A_M , is given by [15]

$$\psi^{sc}(r) = \frac{ike^{ikr}}{4\pi r} \int_{S_M} \left(a\frac{\partial h}{\partial x_0} + b\frac{\partial h}{\partial y_0} - c \right) \times \exp\left(ik[Ax_0 + By_0 + Ch(x_0, y_0)]\right) dx_0 dy_0(1)$$

where

$$A = \sin \theta_{1} - \sin \theta_{2} \cos \phi,$$

$$B = -\sin \theta_{2} \sin \phi,$$

$$C = -(\cos \theta_{1} + \cos \theta_{2}),$$

$$a = \sin \theta_{1} (1 - R_{0}) + \sin \theta_{2} \cos \phi (1 + R_{0}),$$

$$b = \sin \theta_{2} \sin \phi (1 + R_{0}),$$

$$c = \cos \theta_{2} (1 + R_{0}) - \cos \theta_{1} (1 - R_{0}).$$
(2)

The total scattered intensity for isotropic surfaces could be considered as sum of the diffused and coherent parts, the diffused part is [15]

$$\langle I_d \rangle = \frac{k^2 F^2}{2\pi r^2} A_M \exp(-g) \int_0^\infty J_0 \left(kR \sqrt{A^2 + B^2} \right) \times \left[\exp(gCor(R)) - 1 \right] R dR, (3)$$

where $Cor(R) = \frac{\langle h(\mathbf{x}+\mathbf{R})h(\mathbf{x})\rangle}{\sigma^2}$ is the height-height correlation function and $\langle h(\mathbf{x})\rangle = 0$, $g = k^2\sigma^2(\cos\theta_1 + \cos\theta_2)^2$ is the roughness criteria, and $\sigma = \sqrt{\langle (h(\mathbf{x}) - \langle h(\mathbf{x})\rangle)^2\rangle}$ is height root means squared of the rough surface. It is more convenient to write equation (3) in the form

$$\langle \widetilde{I}_d \rangle = \int_0^\infty J_0 \left(kR \sqrt{A^2 + B^2} \right) \times [\exp(gCor(R)) - 1]RdR,$$
 (4)

with $I_d/\widetilde{I}_d=\frac{k^2F^2}{2\pi r^2}A_M \exp(-g)$, where from hereafter the overtilde is omitted. Equation (4) shows the diffused intensity in terms of the height correlation function, where the idea is to find the height correlation function in terms of the diffused intensity. This would be obtained by solving equation (4) making use of the saddle point approximation. Attention must be focused on a few issues; we are considering rough surfaces were $g\gg 1$, this means that the conditions, $k\sigma\gg 1$ and small θ_1 and θ_2 must be fulfilled.

- In highly rough surfaces, $g \gg 1$, the contribution of the coherent term could be neglected in comparison to the contribution of the diffused term, this means that the diffuse intensity I_d would be equal to the total intensity I [15], expressed as

$$I = \int_0^\infty J_0\left(kR\sqrt{A^2 + B^2}\right) \exp(gCor(R))RdR. \quad (5)$$

- In order to satisfy the conditions of the saddle point approximation, the integrand must tend to zero on the integral limits. This condition is not satisfied by Eq. (5), persuading us to differente both side of Eq. (5) in respect to g resulting in

$$\frac{d}{dg}I = \int_0^\infty Cor(R)J_0\left(kR\sqrt{A^2 + B^2}\right) \times \exp(gCor(R))RdR. \tag{6}$$

Note that the derivative has been taken on a path where the Bessel function $J_0(kR\sqrt{A^2+B^2})$ stays constant in respect to the variable g. It could readily be seen that the term $J_0(kR\sqrt{A^2+B^2})$ depends on the wave-length, incident and scattered angles. The Bessel function is kept constant with respect to the variations of g. This is done by keeping the wave-length and incident angle constant and only letting the scattered angles vary in a way to keep the A^2+B^2 constant, see Fig. 2. In Fig. 2, three typical paths corresponding to three different constant values of A^2+B^2 is shown.

Making use of the definition of the logarithmic function we obtain

$$\frac{d}{dg}I = \int_0^\infty J_0\left(kR\sqrt{A^2 + B^2}\right)$$

$$\times \exp\left[g\left(Cor(R) + \frac{\ln(R)}{g} + \frac{\ln(Cor(R))}{g}\right)\right]dR.7$$

Equation (7) would satisfy the conditions for the saddle point approximation, where the argument of the Bessel function must stay constant in respect to g. According to Fig. 2, the variation of θ_2 and ϕ would provide the path where the intensity is measured on. Note that in plotting the curves (paths) of Fig. 2, the Bessel function stays constant with respect to the variations of g.

- To solve the integral of Eq. (7) by the saddle point approximation, Eq. (7) needs to be written in a form

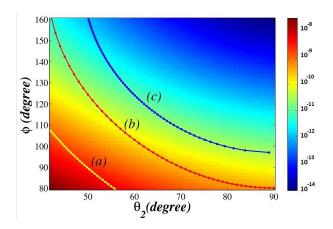


FIG. 2: (Color online) The curves are typical paths on which the Bessel function or A^2+B^2 stays constant with fixed k as g varies. The plane of consideration is the diffused intensity based on the scattered angles θ_2 and ϕ for a Gaussian correlation function. The values for the parameters are; $\theta_1=20^\circ$, $\sigma=50nm$ and $\lambda=500nm$. The paths correspond to (a) $A^2+B^2=0.7$ (b) $A^2+B^2=1$ (c) $A^2+B^2=1.2$.

so how that the extremum would be inside the integral limits and not on the integral limits. By implementing a new variable $u = \ln(R)$, the lower limit of the integral could be changed to $-\infty$. Hence, Eq.(7) would be

$$\frac{d}{dg}I = \int_{-\infty}^{\infty} J_0\left(k\exp(\mathbf{u})\sqrt{A^2 + B^2}\right)$$

$$\times \exp\left[g\left(\widetilde{Cor}(u) + \frac{2u}{g} + \frac{\ln(\widetilde{Cor}(u))}{g}\right)\right]du(8)$$

Since the intensity and intensity variations are needed on the path, and depending on the chosen constant A^2+B^2 , one could refine the correlation. This could be obtained due to the fact that all paths would give a unique height correlation function. This would suggest a new technique for experimentalists to test their obtained results by choosing specific incident angles, incident wave-lengths, to keep the desired J_0 constant in respect to g. In other words to keep J_0 constant, the parameter A^2+B^2 must stay constant. In this way a new path may be suggested for finding the intensity experimentally. Fig. 2 shows three paths obtained for three constant values of A^2+B^2 , $\theta_1=20^0$ and $\lambda=500\,nm$.

In this stage Eq. (8) complies the saddle point approximation by

$$f(u) = \widetilde{Cor}(u) + \frac{2u}{g} + \frac{\ln(\widetilde{Cor}(u))}{g},$$

$$f'(u^*) = \widetilde{Cor}'(u^*) + \frac{2}{g} + \frac{\widetilde{Cor}'(u^*)}{g\widetilde{Cor}(u^*)} = 0,$$

$$f''(u^*) = \widetilde{Cor}''(u^*) + \frac{1}{g} \frac{\widetilde{Cor}''(u^*)\widetilde{Cor}(u^*) - \widetilde{Cor}'^2(u^*)}{\widetilde{Cor}^2(u^*)}$$

where, u^* is the desired saddle point. Solving the integral in equation (8) by the saddle point approximation gives

$$\frac{d}{dg}I = \sqrt{2\pi}J_0\left(k\exp(u^*)\sqrt{A^2 + B^2}\right)$$
$$(gf''(u^*))^{-\frac{1}{2}}\exp(gf(u^*)), \tag{10}$$

due to the complexity of the RHS of Eq. (10), an explicit version for the height correlation function may not be obtained without the use of the second derivative of Eq. (8)

$$\frac{d^2}{dg^2}I = \widetilde{Cor}(u^*)\sqrt{2\pi}J_0\left(k\exp(u^*)\sqrt{A^2 + B^2}\right)$$

$$(gf''(u^*))^{-\frac{1}{2}}\exp(gf(u^*)), \tag{11}$$

Equation (11) is an expression in terms of Cor(u) in the extremum point which itself is dependent on g. This means that changing g by differing the wave-length, standard deviation, incident and scattering angles, the correlation function would vary. This enables us to obtain the functionality of the correlation on g instead of just having a specific point. By dividing both sides of Eqs. (10) and (11), the expression for $Cor(u^*)$ is obtained

$$\widetilde{Cor}(u^*) = \frac{\frac{d^2}{dg^2}[I]}{\frac{d}{dg}[I]} = W(g). \tag{12}$$

Equation (12) shows the relation between $\widetilde{Cor}(u^*)$ and g. Due to the fact that W(g) could be observed experimentally, Eq. (12) would give the correlation function. But the issue which still remains is the value of u^* .

From the second expression of Eq. (9) an explicit relation between the derivative of the height correlation and g for the limiting case of highly rough surfaces ($g \gg 1$) is obtained

$$\widetilde{Cor}'(u^*) = -\frac{2}{g + \frac{1}{\widetilde{Cor}(u^*)}} \simeq -\frac{2}{g}.$$
 (13)

The derivative of Eq. (12) with respect to g would show the functionality of u^* in terms of g

$$\frac{d\widetilde{Cor}(u^*)}{dg} = \frac{du^*}{dg}\widetilde{Cor}'(u^*) = \frac{dW(g)}{dg},\tag{14}$$

and by using Eq. (13)

$$u^*(g) = -\int \frac{g}{2} \frac{dW(g)}{dq} dg, \qquad (15)$$

which with partial integration, it could be obtained $u^*(q)$

$$u^*(g) = -\frac{gW(g)}{2} + \int \frac{W(g)}{2} dg.$$
 (16)

Equation (16) gives an expression for u^* on g. The relation between $\widetilde{Cor}(u^*)$ with g is already shown in Eq.

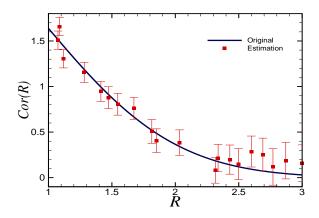


FIG. 3: Comparison of the correlation function estimated by the PDSW model and the original exponential correlations. The parameters for this estimation are; $A^2 + B^2 = 0.8$, $\theta_1 = 20^{\circ}$, $\sigma = 0.5$ and $k\sigma = 1.2$.

(12), so the dependence of the height correlation function on u may readily be obtained. Since $u = \ln(R)$, the dependence of the height correlation function on R may be obtained.

The procedure could be illustrated as follows; incident light with a specific angle to a rough surface with a constant wave length (preferably small) scatters with a verity of angles. The measured intensity for each scattered angle on the desired path needs to be differentiated in respect to g (which depends on the scattered angle) twice. Then the ratio of the second derivative and the first derivative is obtained in order to find W(g). Substituting W(g) in Eq. (16) the parameter $u^*(g)$ is obtained, keeping in mind that W(g) is the height correlation of u^* . Having the dependence or in other words variations of $\widehat{Cor}(u^*)$ and u^* on g the height correlation on R is obtained.

In Fig. 3 the applicability and robustness of this technique is illustrated. Where as an example we estimate the known exponential correlation function with the PDSW model and compare it with the original cases showing a very good consistency. The parameters for this estimation are; $A^2 + B^2 = 0.8$, $\theta = 20^{\circ}$, $\sigma = 0.5$ and $k\sigma = 1.2$.

The applicability of the method introduced in this work for experimentalists although has a very simple procedure, would give the height correlation function of the surface. The height correlation function is the most important feature in order to understand the physics of a rough surface which is applicable to various fields of physics. "The path derivative scattered wave" introduced in this work would prove as an easy to use technique for experimentalists since only by measuring the intensity of the scattered light on a specific path, the height correlation function of a specific rough surface could be obtained.

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